Biomarkers in herbicide exposed plants

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Figure S1. Flowchart of the chemical and data analysis.

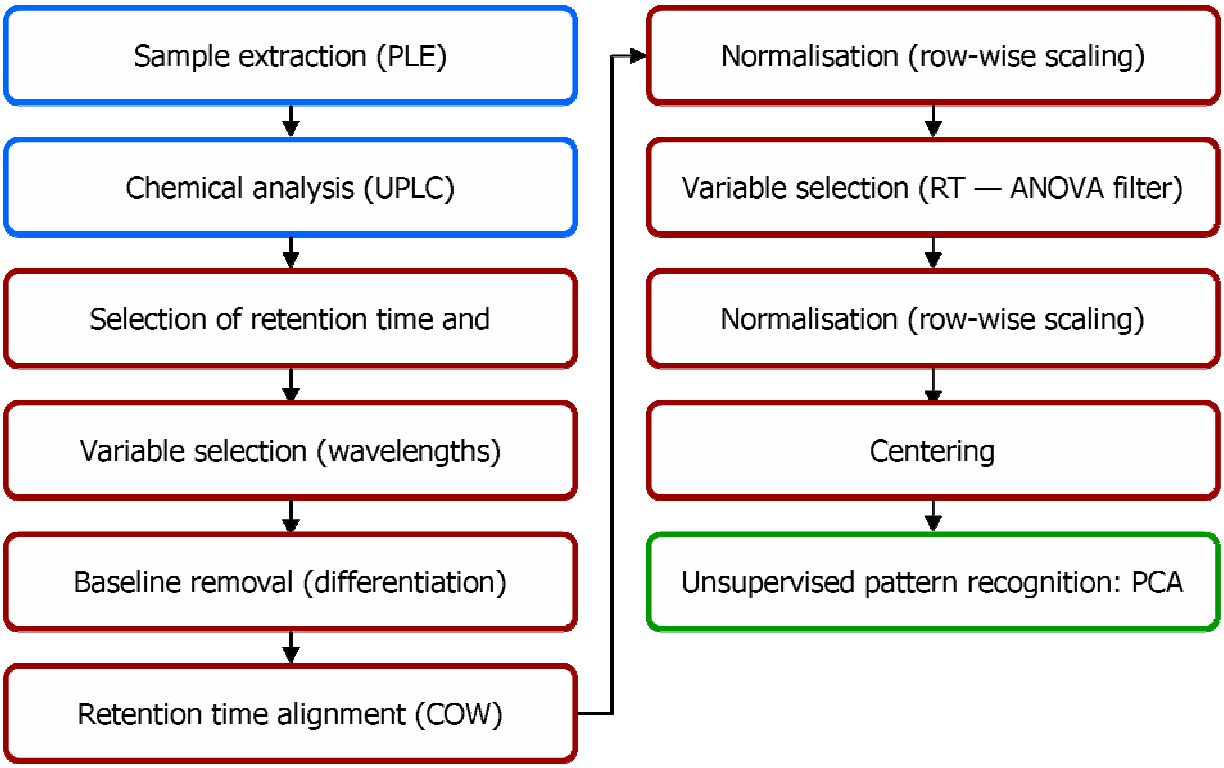
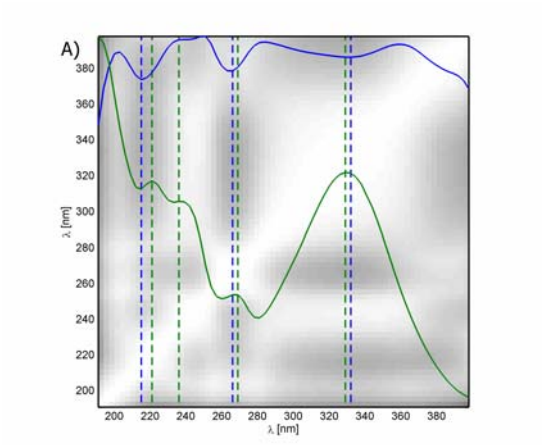
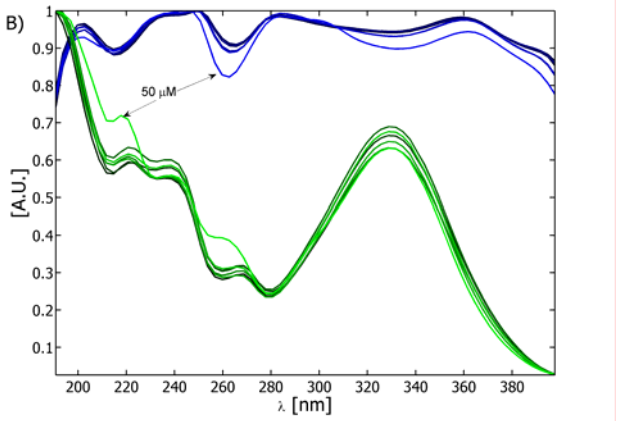


Figure S2 Results of the initial wavelength selection. A) Matrix of correlation coefficients for the four biological replicates of plants exposed to 10 µM glyphosate with overlaid the sum of correlation coefficients (*r*, in blue) and the variance (*s*, in green) of each wavelength. The darker the colour, the lower is the correlation between the corresponding wavelengths. Four groups of variables are clearly visible (white parts, corresponding to a correlation ≥ 0.9) centered around the selected wavelengths. Note also that the *r* and *s* curves are normalised to have maximum equal to one. The dashed lines correspond to local minima and maxima of *r* and *s* respectively. B) *r* and *s* curves (again normalised to maximum equal to 1) for the seven exposure levels (lighter colour means higher exposure). C) Sum of frequencies of selection for *r* and *s*. The ordinate axis in C denotes the sum of the selection rates across exposures for both *r* and *s*. Therefore 2 means that the wavelength is selected for both dissimilarity and variance measure in all the cases at all the exposure levels.





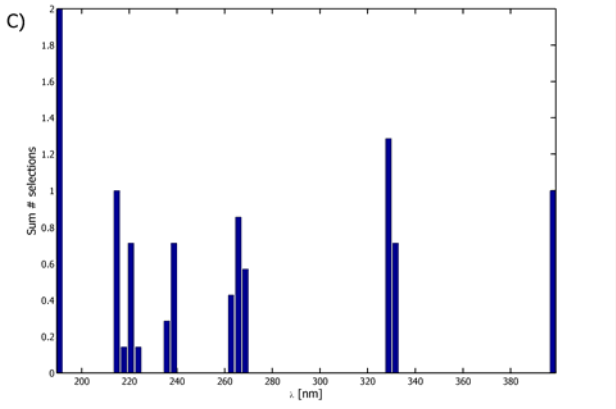


Figure S3. Picture of the 28 plants. The exposure increases from right to left. As can be observed, the one of the 30µM plants look considerably less affected than the other replicates.

Figure S4. RMSECV for the choice of *v* and *K*.

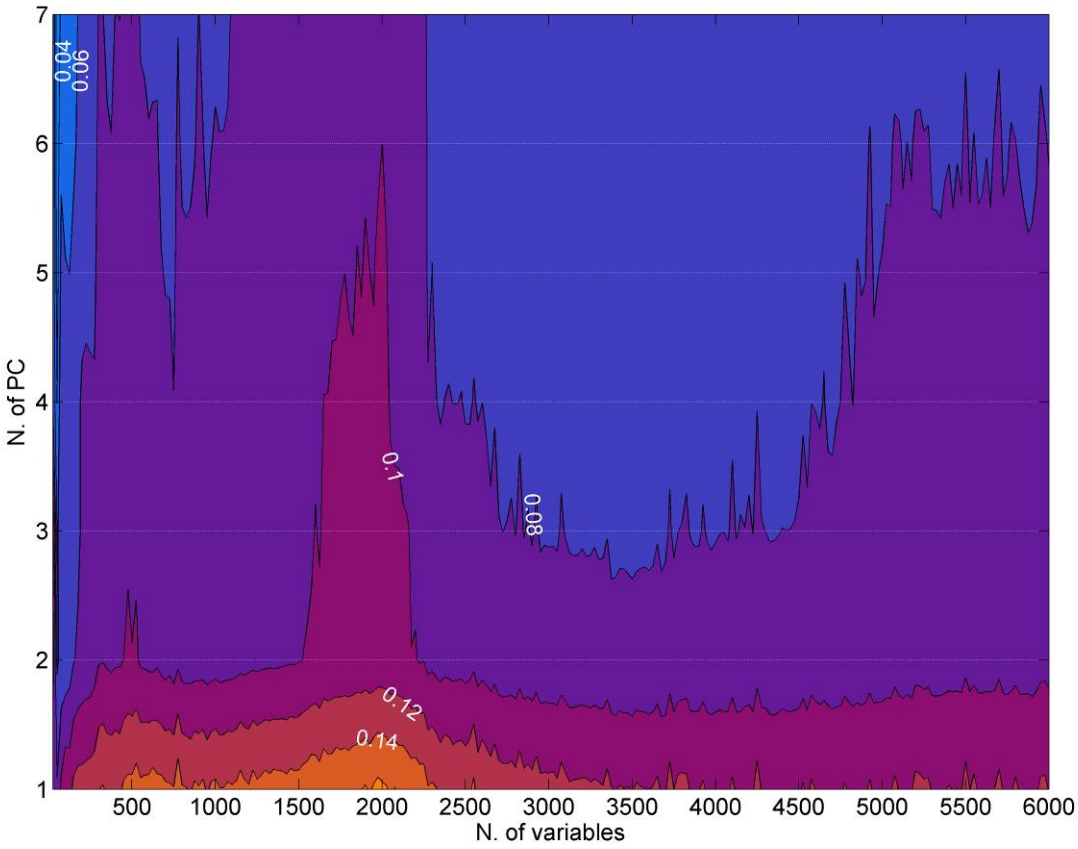


Figure S5. Linear discriminant analysis of the controls plus the 1µM samples vs. the 5 µM + 10 µM for five choices of *v*: A) 50, B) 500, D) 3400. Circles represent the analytical replicates classified according to the main sample set. Diamonds represent the independent test set.

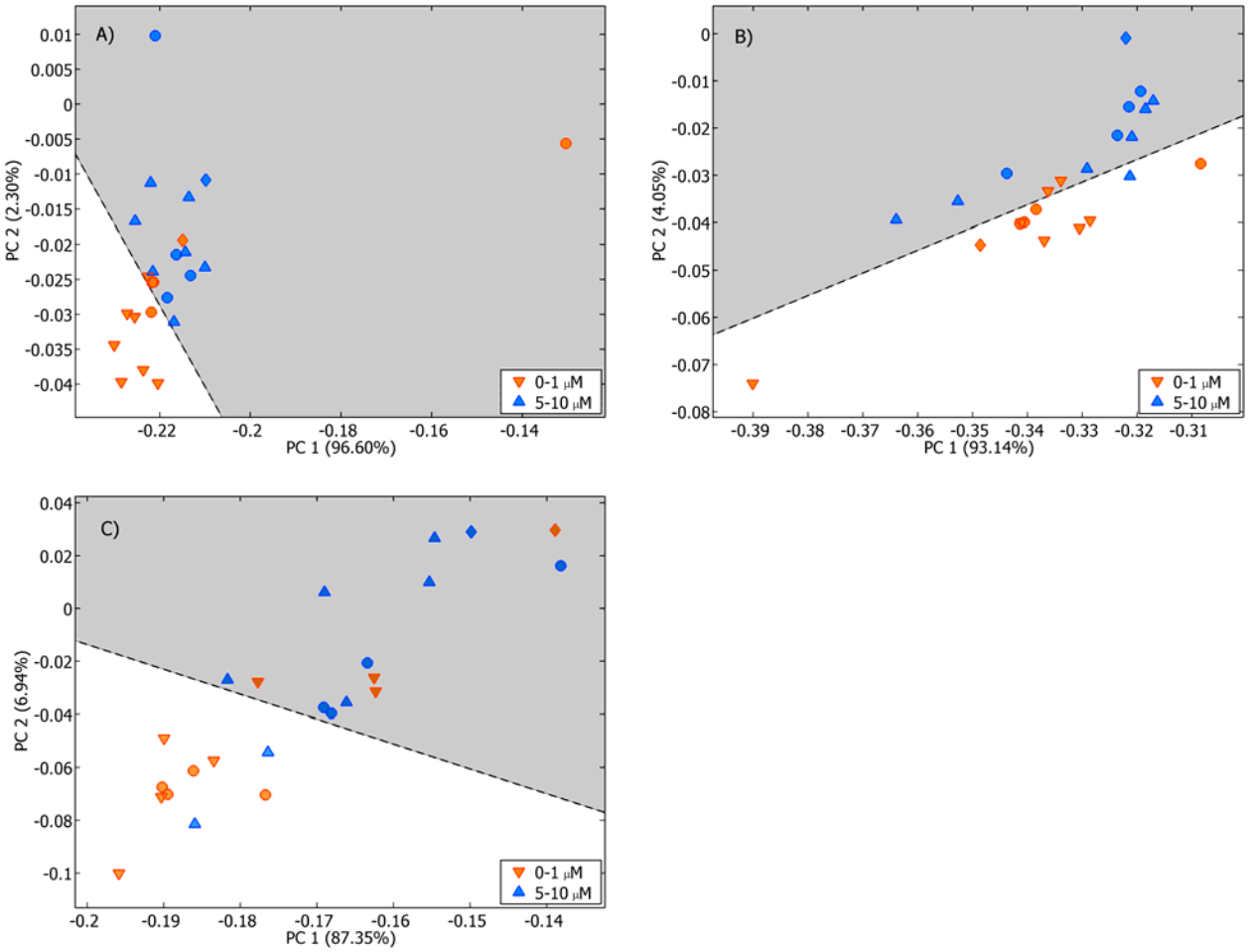
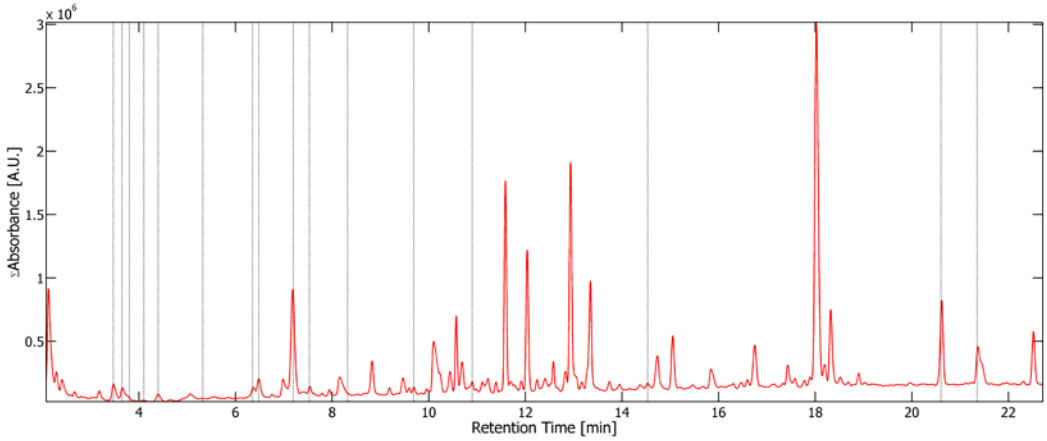


Figure S6. Peaks with large coefficients for either PC1 or PC2 in the 500 variables model. In red, the sum of the four selected wavelengths for a reference set sample (upper figure).



Zoom of the relevant peak regions (left hand side) and UV-VIS spectra of the marked retention times (right hand side)

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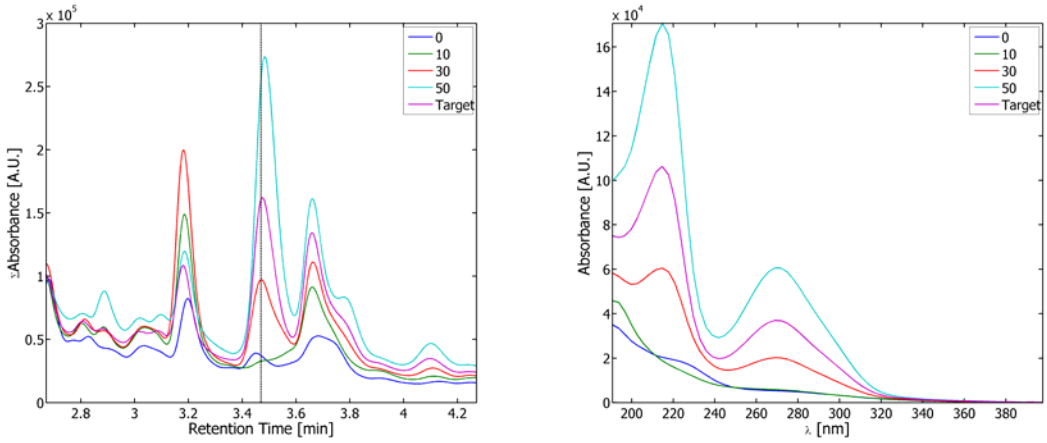

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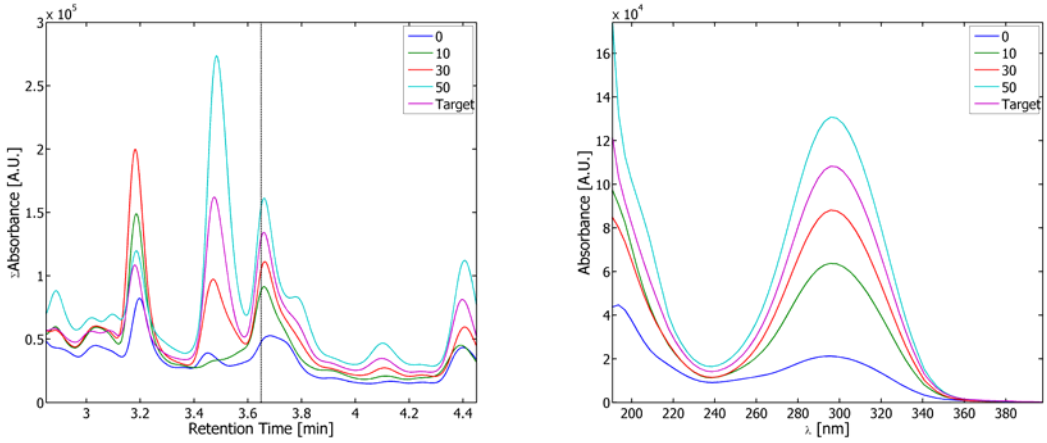

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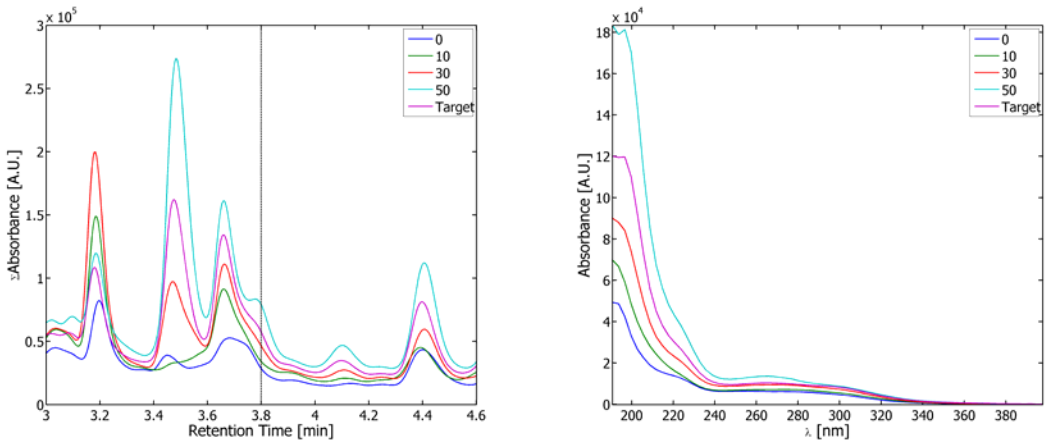
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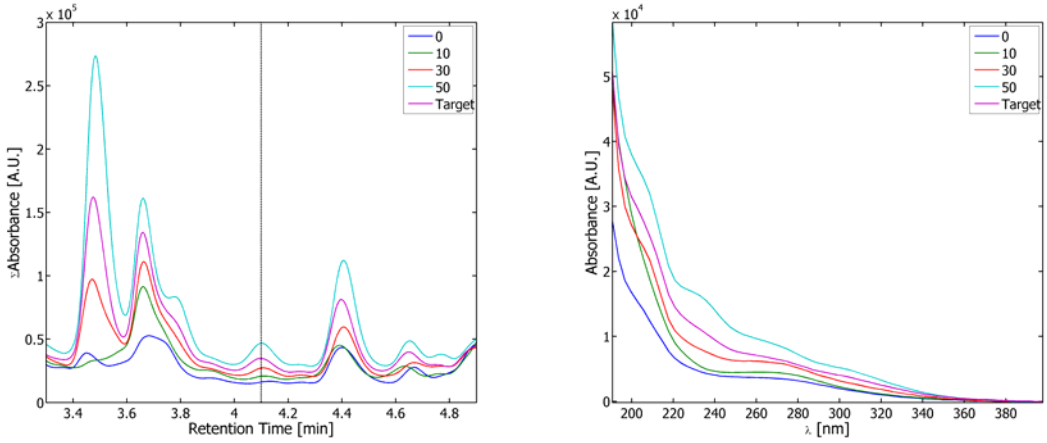
0
10
30
50
Target
x 10^4
Absorbance [A.U.]
λ [nm]

4.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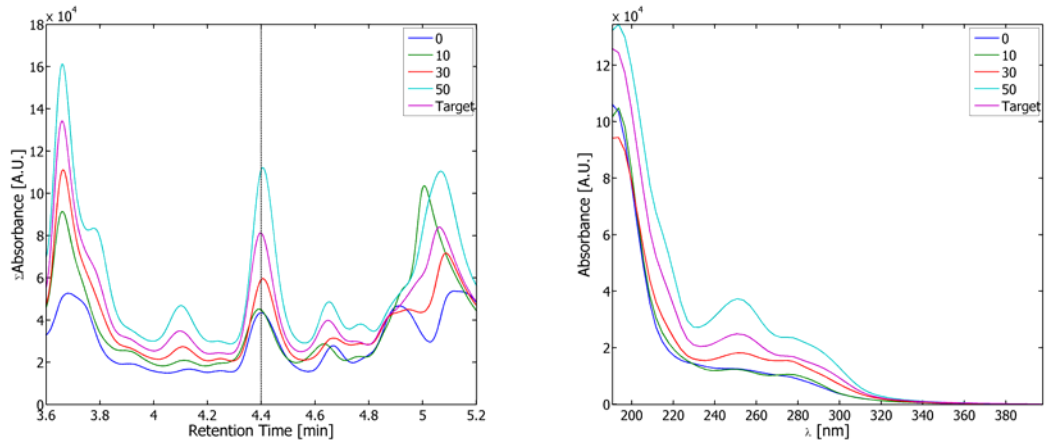
x 10^4
Absorbance [A.U.]
λ [nm]

5.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Absorbance [A.U.]
λ [nm]

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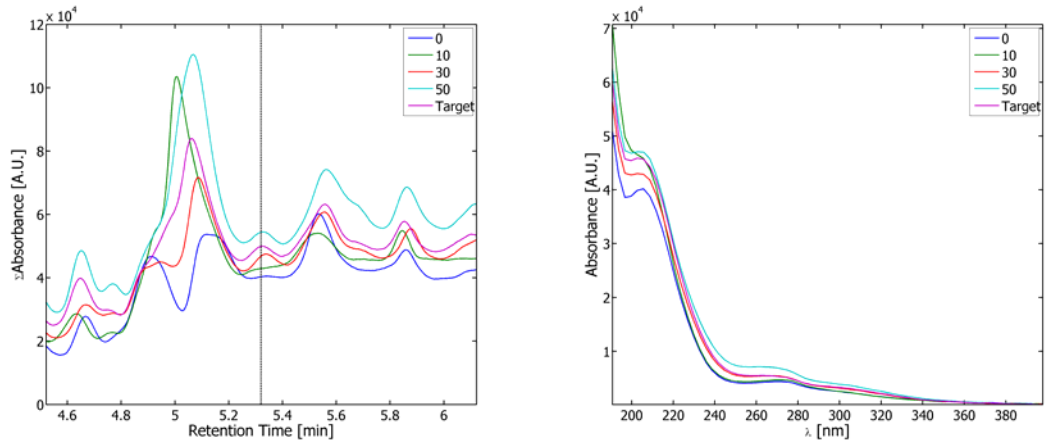
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Target
x 10^4
Absorbance [A.U.]
λ [nm]

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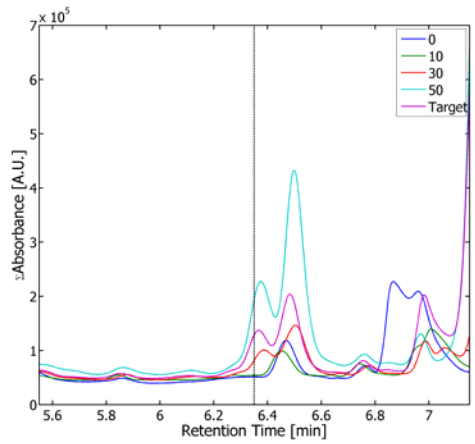
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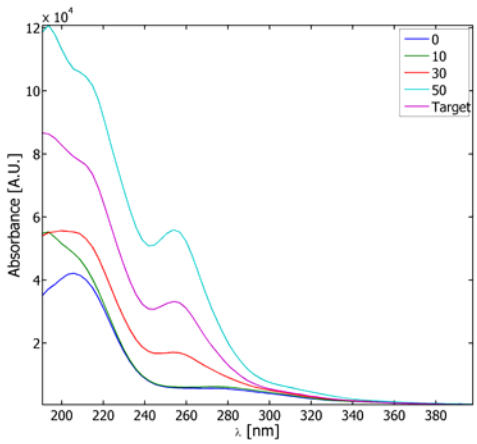
Target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λ [nm]
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Target

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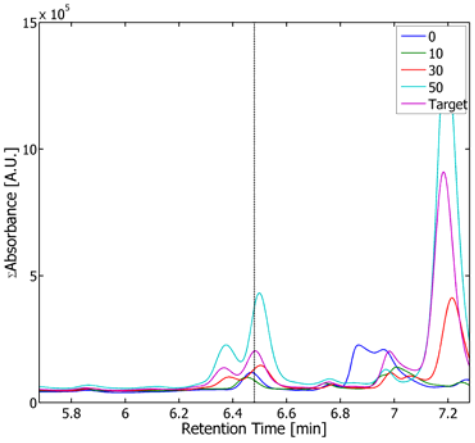
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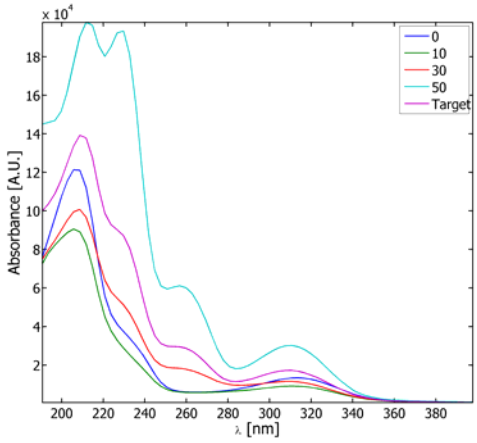
Target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λ [nm]
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Target

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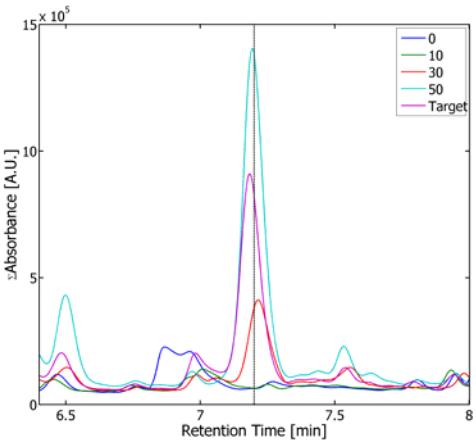
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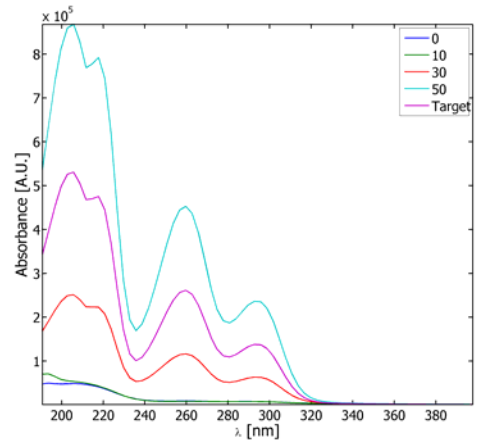
Target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λ [nm]
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Target

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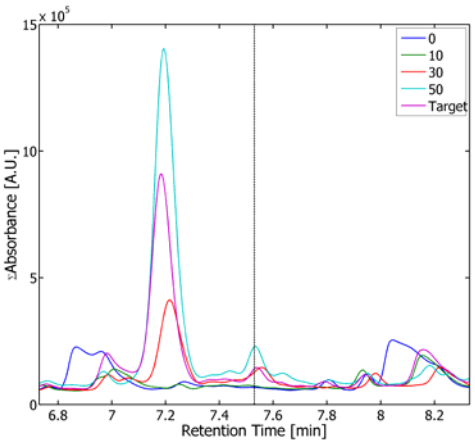
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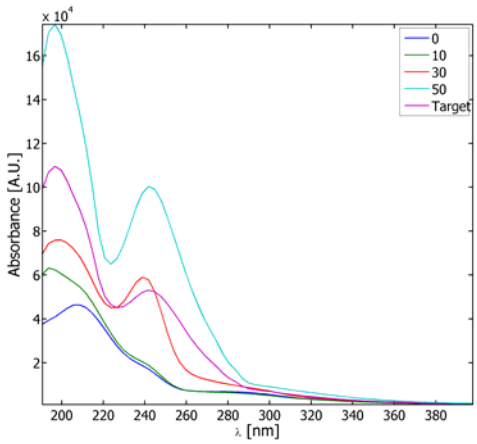
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λ [nm]
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Target

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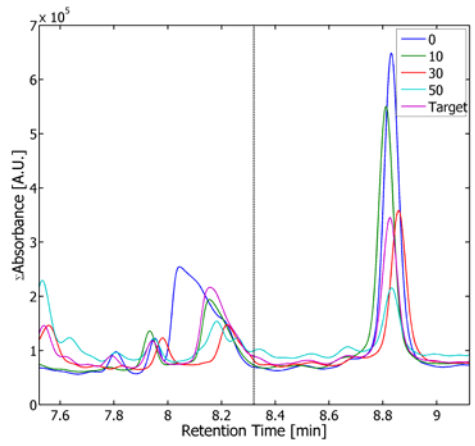
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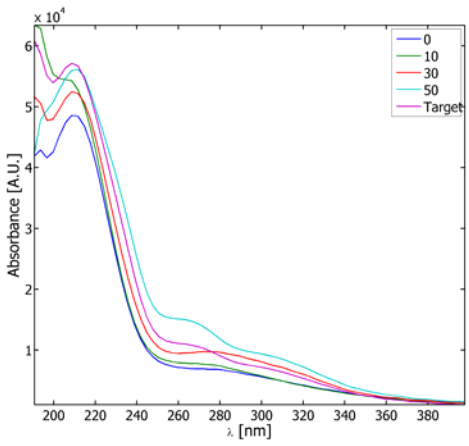
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λ [nm]
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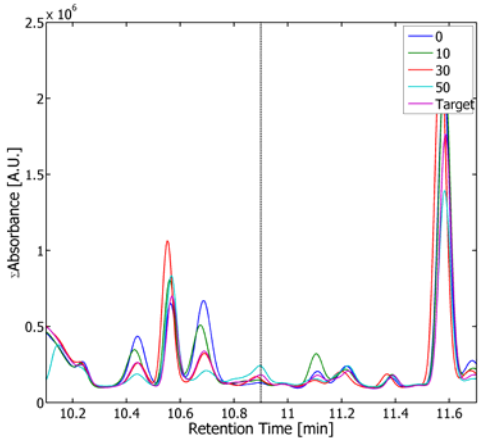
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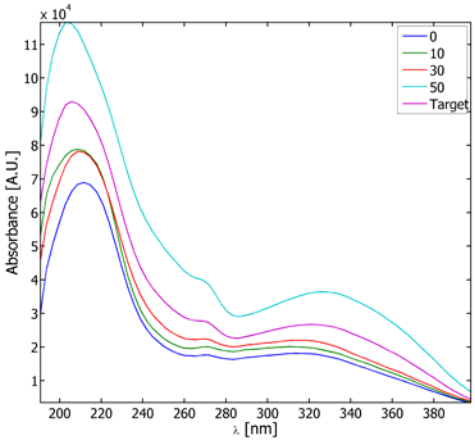
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Target

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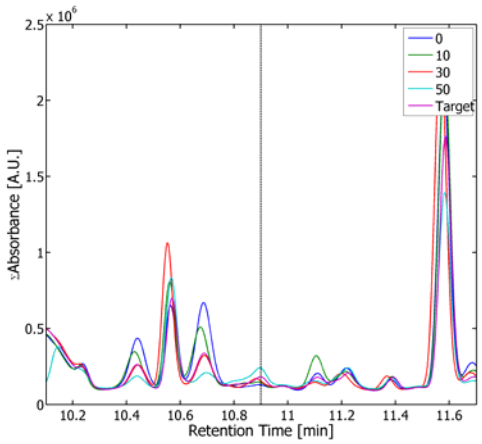
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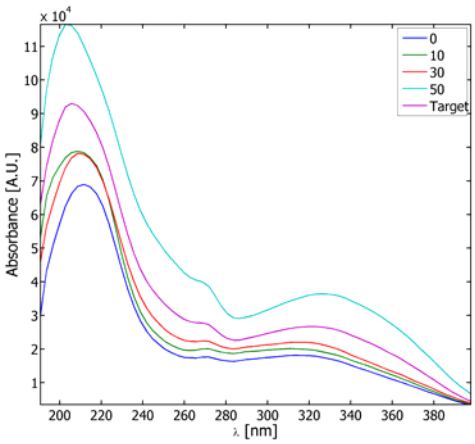
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λ [nm]
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30
50
Target

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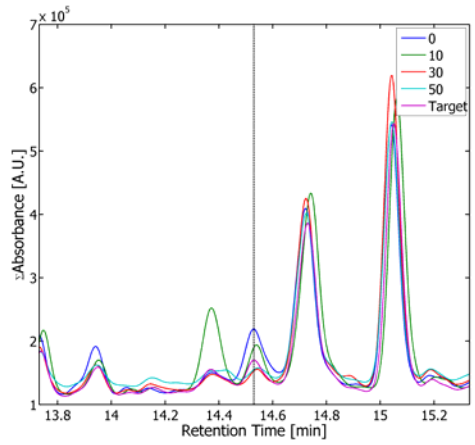
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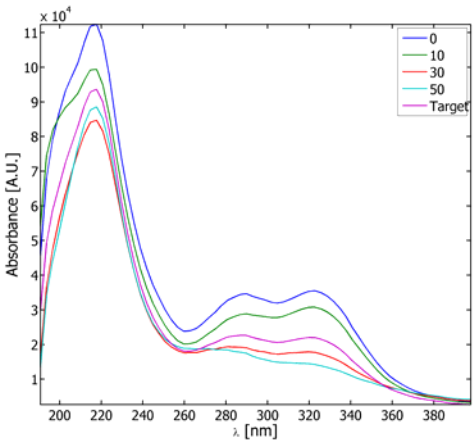
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λ [nm]
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10
30
50
Target

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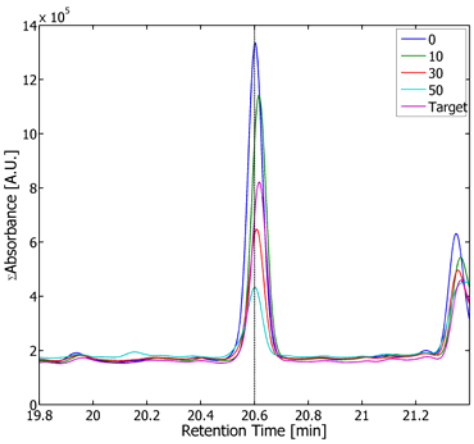
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Σ Absorbance [A.U.]
Retention Time [min]
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10
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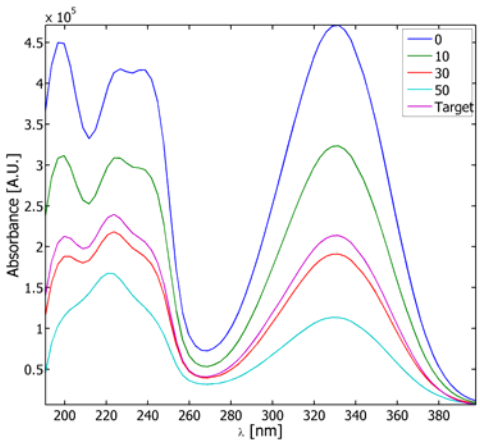
Target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Absorbance [A.U.]
λ [nm]
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10
30
50
Target

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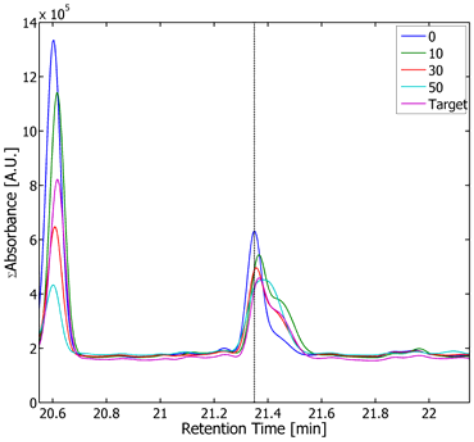
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Σ Absorbance [A.U.]
Retention Time [min]
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10
30
50
Target

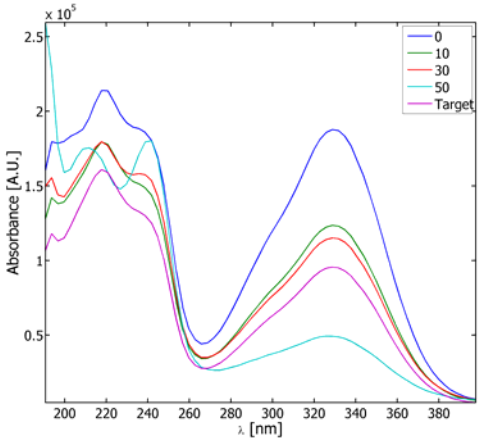
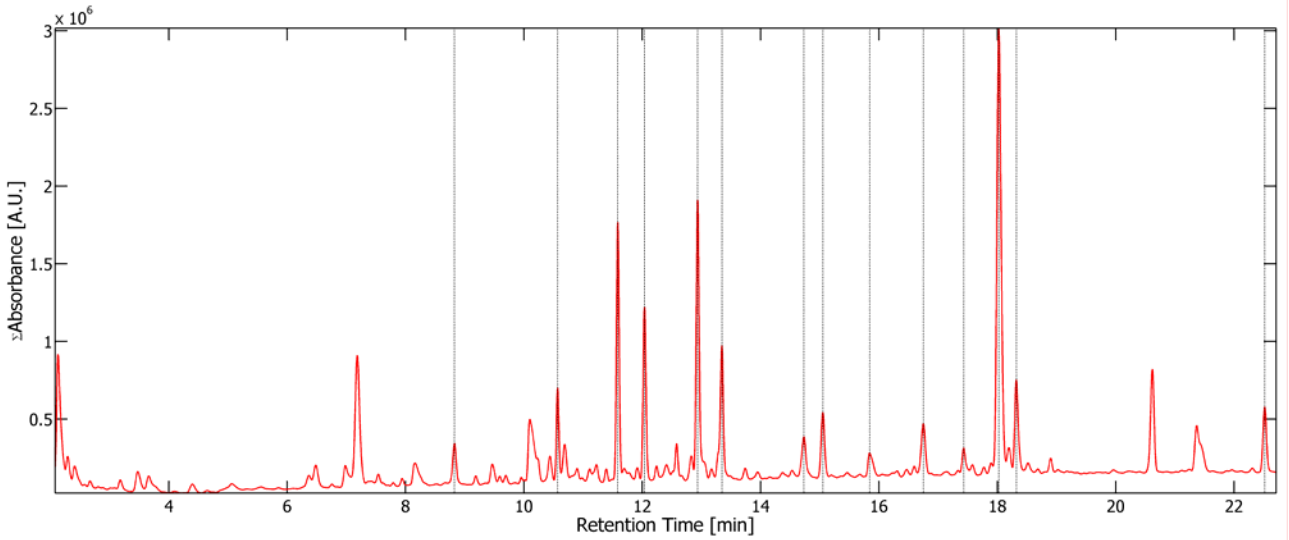

x 10^5
Absorbance [A.U.]
λ [nm]
0
10
30
50
Target

Figure S7. Large peaks with small loading coefficients for PC1 and PC2 in the 500 variables model. In red, the sum of the four selected wavelengths for a reference set sample (upper figure).



Zoom of the peak regions (left hand side) and UV-VIS spectra of the marked retention times (right hand side)

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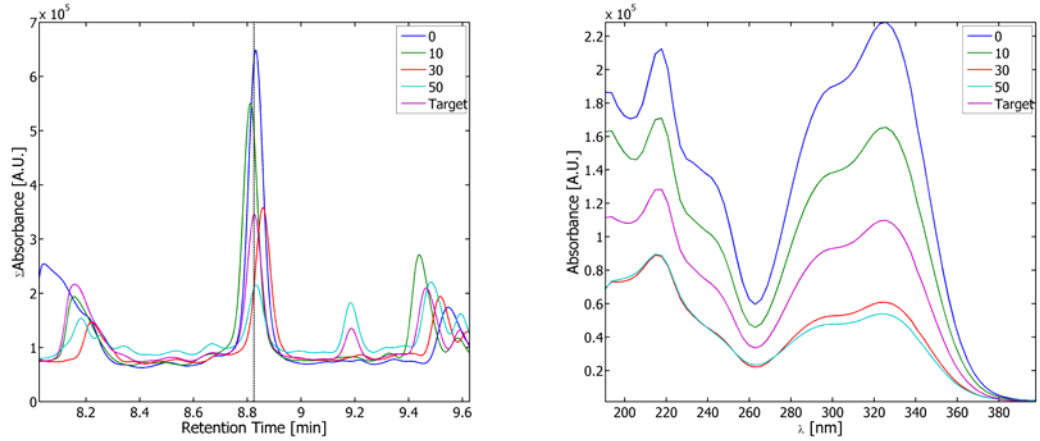

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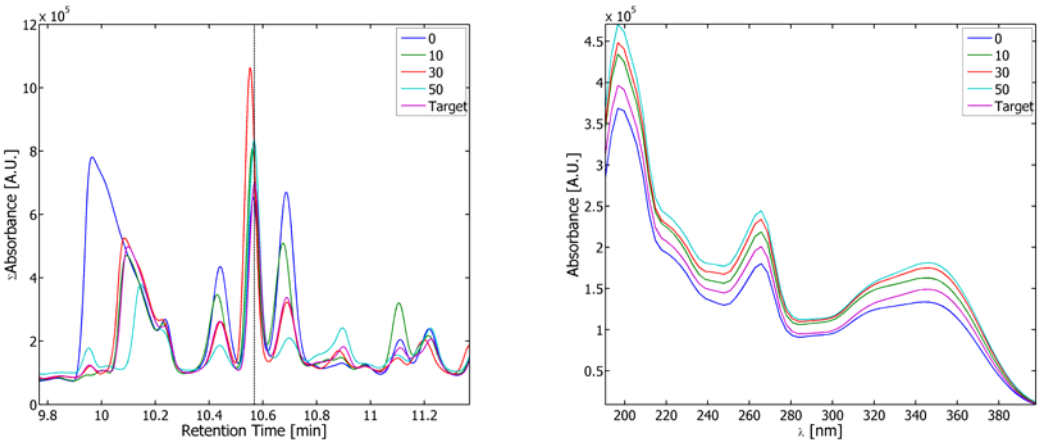

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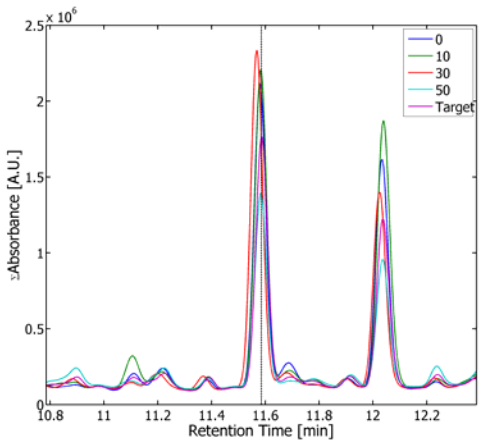
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Σ Absorbance [A.U.]
Retention Time [min]
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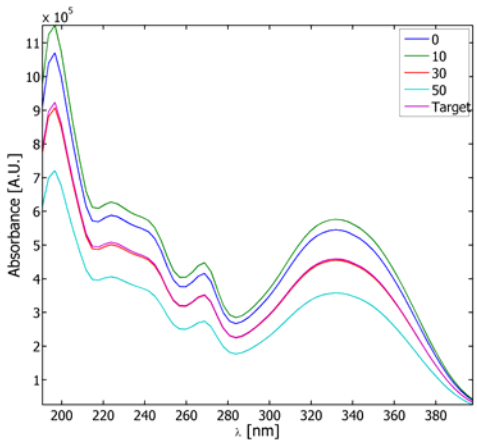
10
30
50
Target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Absorbance [A.U.]
λ [nm]
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30
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Target

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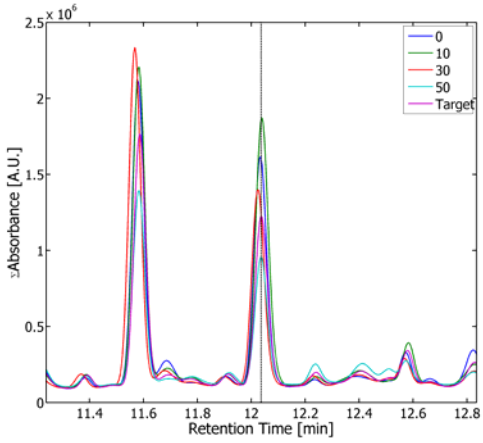
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Retention Time [min]
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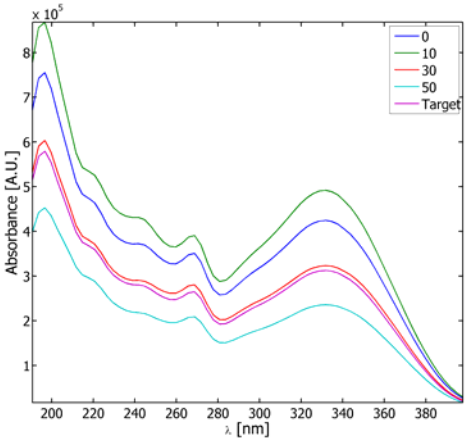
10
30
50
Target


x 10^5
Absorbance [A.U.]
λ [nm]
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30
50
Target

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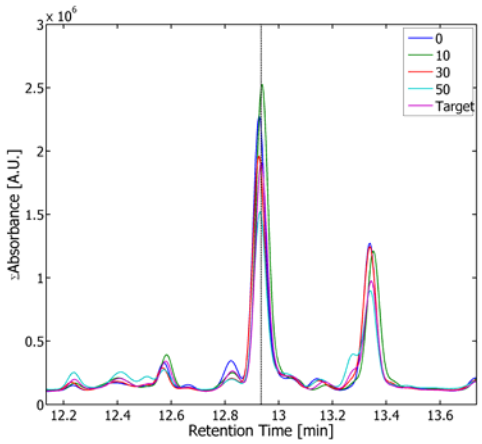
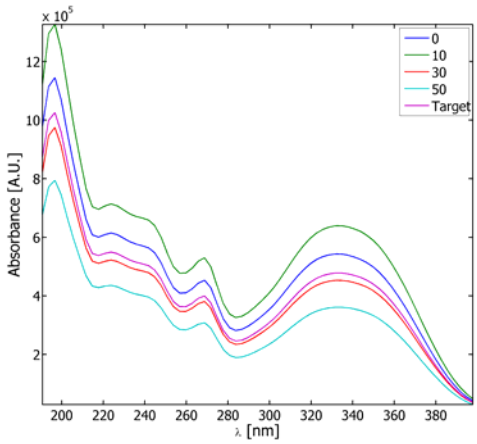
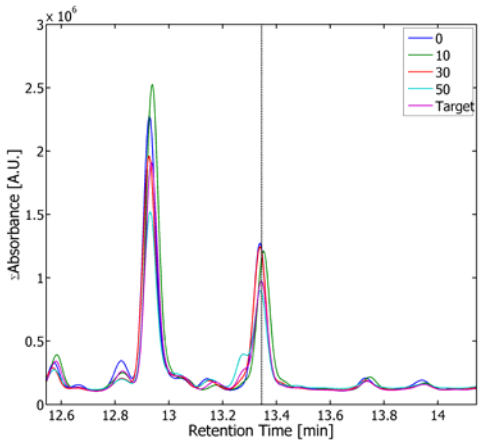
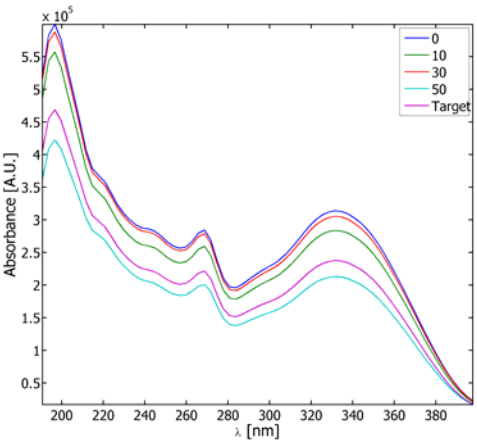

x 10^6
Σ Absorbance [A.U.]
Retention Time [min]
0
10
30
50
Target

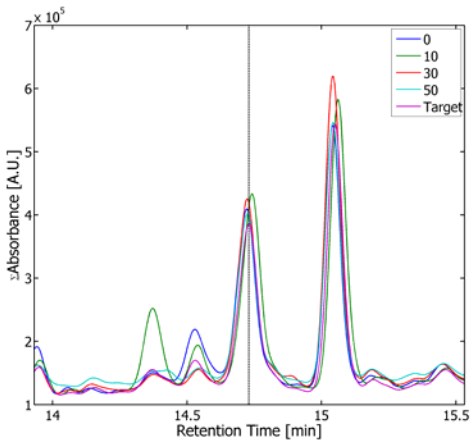

x 10^5
Absorbance [A.U.]
λ [nm]
0
10
30
50
Target

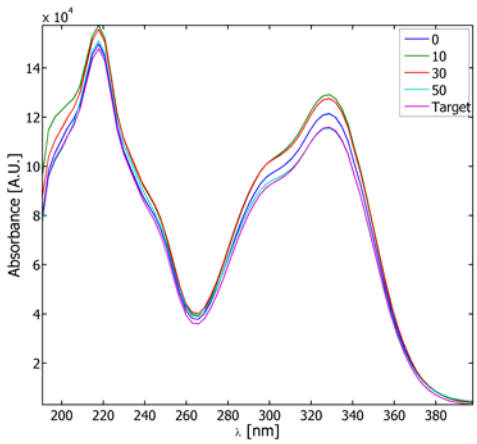
6.


x 10^6
Σ Absorbance [A.U.]
Retention Time [min]
0
10
30
50
Target

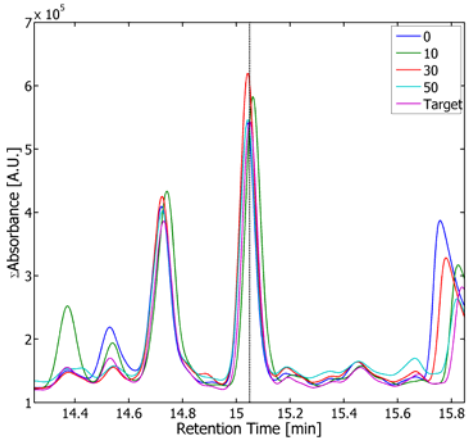

x 10^5
Absorbance [A.U.]
λ [nm]
0
10
30
50
Target

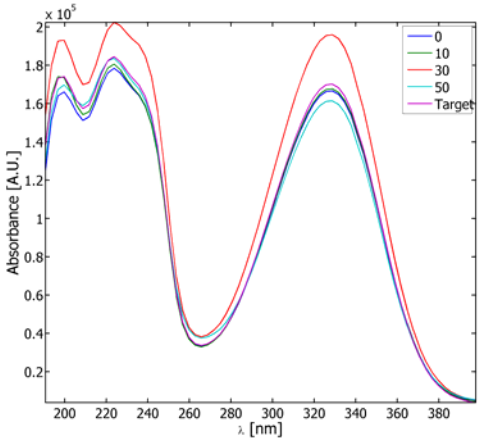
7.


x 10^5
Absorbance [A.U.]
Retention Time [min]
0
10
30
50
Target

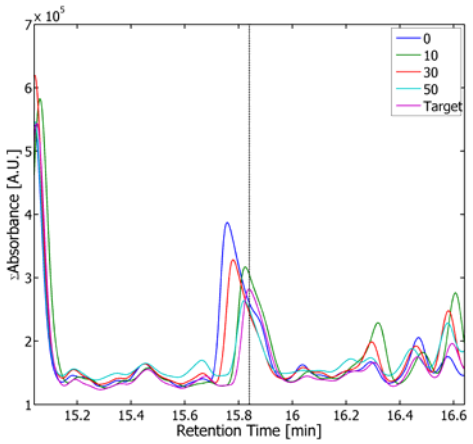

x 10^4
Absorbance [A.U.]
λ [nm]
0
10
30
50
Target

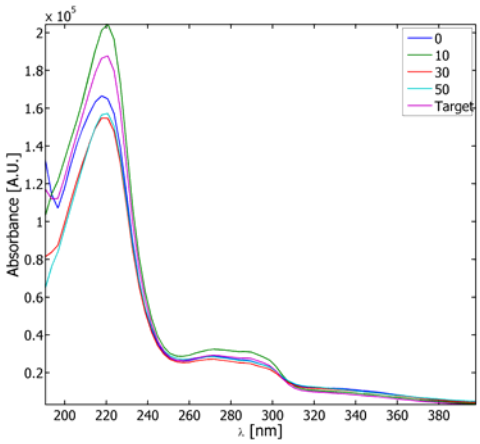
8.


x 10^5
Absorbance [A.U.]
Retention Time [min]
0
10
30
50
Target

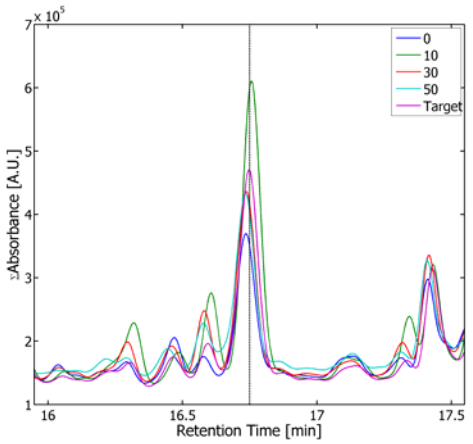

x 10^5
Absorbance [A.U.]
λ [nm]
0
10
30
50
Target

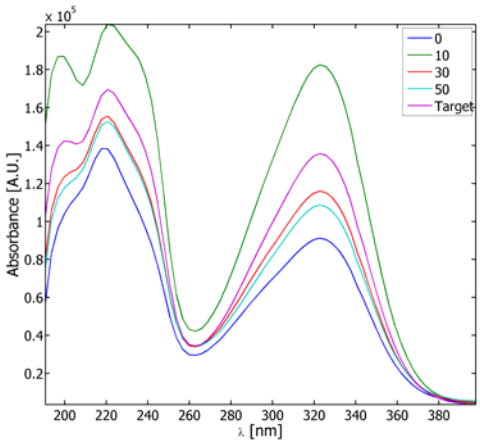
9.


x 10^5
Absorbance [A.U.]
Retention Time [min]
0
10
30
50
Target

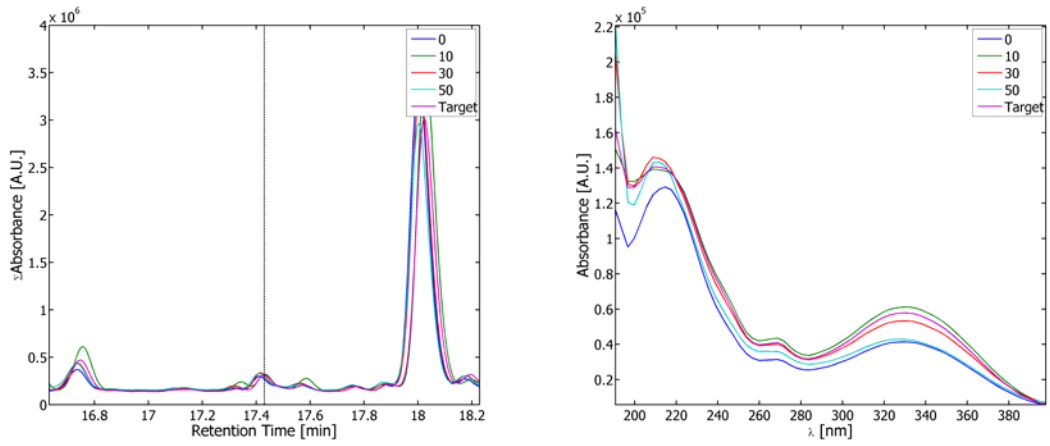

x 10^5
Absorbance [A.U.]
λ [nm]
0
10
30
50
Target

10.

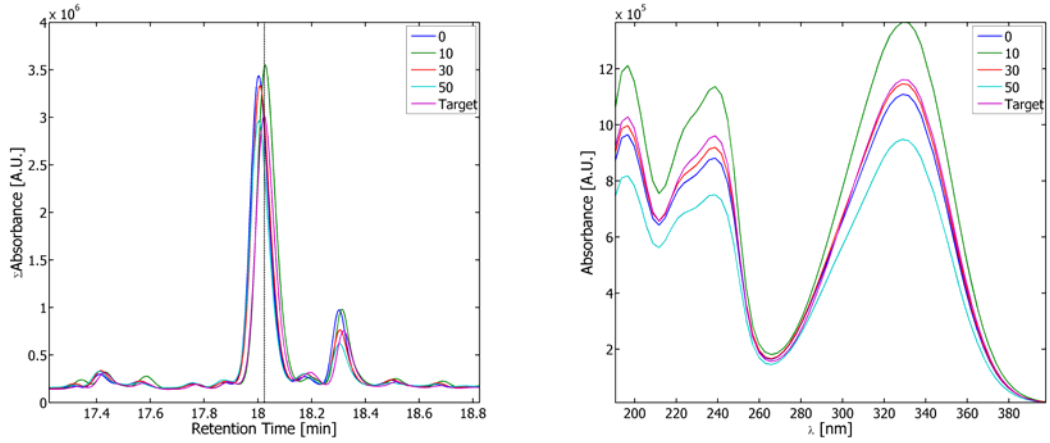

x 10^5
Absorbance [A.U.]
Retention Time [min]
0
10
30
50
Target


x 10^5
Absorbance [A.U.]
λ [nm]
0
10
30
50
Target

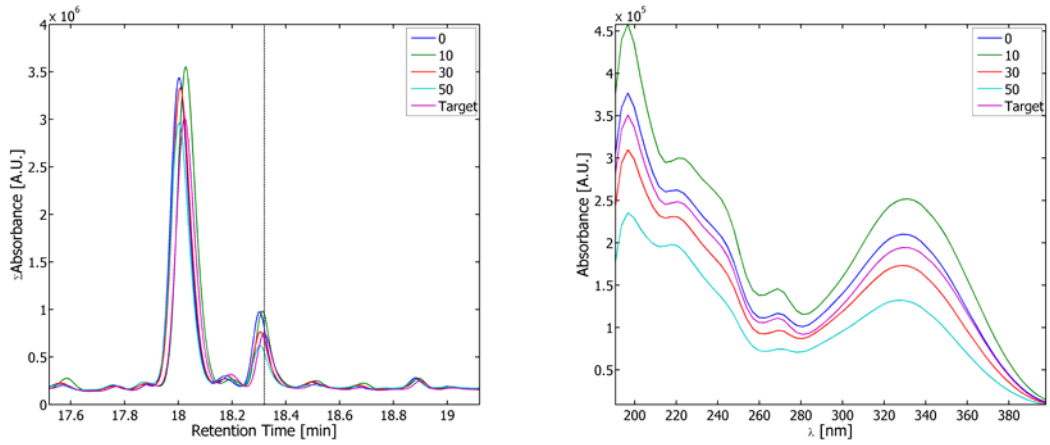
11.


x 10^6
Σ Absorbance [A.U.]
Retention Time [min]
0
10
30
50
Target
x 10^5
Absorbance [A.U.]
λ [nm]

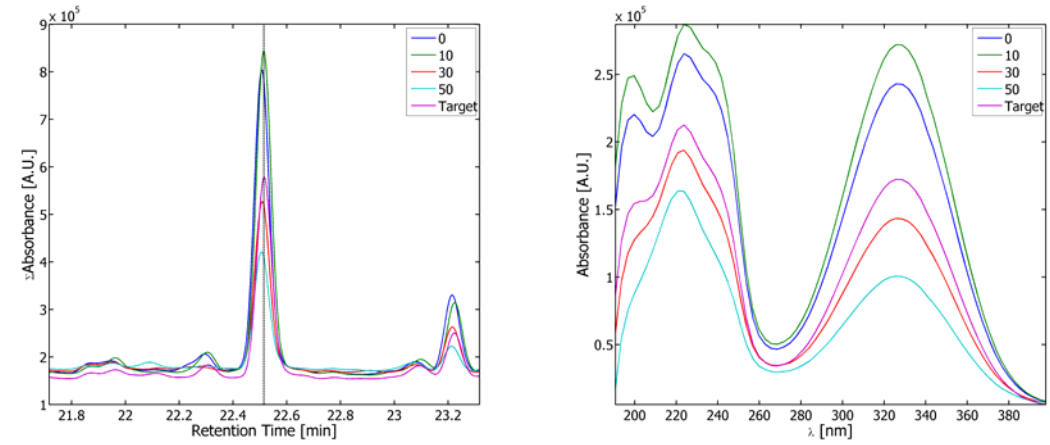
12.


x 10^6
Σ Absorbance [A.U.]
Retention Time [min]
0
10
30
50
Target
x 10^5
Absorbance [A.U.]
λ [nm]

13.


x 10^6
Σ Absorbance [A.U.]
Retention Time [min]
0
10
30
50
Target
x 10^5
Absorbance [A.U.]
λ [nm]

14.


x 10^5
Σ Absorbance [A.U.]
Retention Time [min]
0
10
30
50
Target
x 10^5
Absorbance [A.U.]
λ [nm]